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Patent and Trademark Office; U.S. DEPARTMENT OF COMMERCE

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Attorney Docket Number 426.97.265 **DECLARATION FOR UTILITY OR** DeWitte First Named Inventor DESIGN COMPLETE IF KNOWN PATENT APPLICATION (37 CFR 1.63) 09 220,363 Application Number December 24, 1998 Filing Date ☐ Declaration ■ Declaration OR Not Assigned Submitted Submitted after Initial Group Art Unit with Initial Filing (surcharge (37 CFR 1.16 (e)) Filing **Examiner Name** Not Assigned

As a below named inve	ntor, I hereby declare that:					
My residence, post office address, and citizenship are as stated below next to my name.						
I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:						
System and Method for Structure-Based Drug Design That						
Includes A	ccurate Predict	tion of Binding	g Free En	ergy		
the specification of which (Title of the invention).						
is attached hereto						
was filed on (MM/E	12/24/98	as Unite	d States Applica	ation Number or I	PCT International	
Application Number 0	9/220,363 and w	as amended on (MM/DD/Y	m)		(il applicable).	
	eviewed and understand the		titled specification	on, including the	daims, as	
	ent specifically referred to ab		4.44127.01	-0.454		
I acknowledge the duty to d	disclose Information which is	material to pateriability as	defined in 37 Ci	-H 1.56.		
I hereby claim foreign priority benefits under 35 U.S.C. 119(a)-(d) or 365(b) of any foreign application(s) for patent or inventor's certificate, or 365(a) of any PCT international application which designated at least one country other than the United States of America, listed below and have also identified below, by checking the box, any foreign application for patent or inventor's certificate, or of any PCT international application having a filling date before that of the application on which priority is claimed.						
Prior Foreign Application Number(s)	Country	Foreign Filing Date (MM/DD/YYYY)	Priority Not Claimed	Certified Co YES	py Attached? NO	
			0000	0000	0000	
Additional foreign application numbers are listed on a supplemental priority data sheet PTO/SB/02B attached hereto:						
	nder 35 U.S.C. 119(e) of an					
Application Number	(s) Filing Date	(MM/DD/YYYY)			l	
				nal provisional		
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				B/02B attache		

[Page 1 of 4]

Burden Hour Statement: This form is estimated to take 0.4 hours to complete. Time will vary depending upon the needs of the individual case, Any comments on the amount of time you are required to complete this form should be sent to the Chief Information Officer, Patent and Trademark Office, Washington, DC 20231. D NOT SEND FEES OR COMPLETED FORMS TO THIS ADDRESS. SEND TO: Assistant Commissioner for Patents, Washington, DC 20231.

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DECLARATION — Utility or Design Patent Application

I hereby claim the benefit under 35 U.S.C. 120 of any United States application(s), or 365(c) of any PCT international application designating the United States of America, listed below and, insofar as the subject matter of each of the claims of this application is not disclosed in the prior United States or PCT International application in the manner provided by the first paragraph of 35 U.S.C. 112, I acknowledge the duty to disclose information which is material to patentability as defined in 37 CFR 1.56 which became available between the filing date of the prior application and the national or PCT international filing date of this application. **U.S. Parent Application or PCT Parent Parent Patent Number** Parent Filing Date Number (MM/DD/YYYY) (if applicable) 08/741,866 09/26/96 Additional U.S. or PCT International application numbers are listed on a supplemental priority data sheet PTO/SB/028 attached hereto. As a named inventor, I hereby appoint the following registered practitioner(s) to prosecute this application and to transact all business in the Paten and Trademark Office connected therewith: Customer Number Place Customer Number Bar Code OR Registered practitioner(s) name/registration number listed below I abel here Registration Registration Name Number Number Keum J. Park 42,059 XI Additional registered practitioner(s) named on supplemental Registered Practitioner Information sheet PTO/SB/02C attached hereto. Direct all correspondence to: Customer Number OR X Correspondence address below or Bar Code Label Keum J. Park Name Hale and Dorr LLP Address 60 State Street Address Boston MA 02109 City State ZIP Telephone 617-526-6110 USA 617-526-5000 Country Fay I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under 18 U.S.C. 1001 and that such willful false statements may jeopardize the validity of the application or any patent issued thereon. A petition has been filed for this unsigned inventor Name of Sole or First Inventor: Given Name (first and middle [if any]) Family Name or Sumame Robert DeWitte inventor's Date Signature Gurnee ILUSA Canada Residence: City Citizenship 1518 Almaden Lane Post Office Address Post Office Address 60031 Gurnee USA Country

_supplemental Additional Inventor(s) sheet(s) PTO/SB/02A attached hereto

X Additional inventors are being named on the 1

PTO/SB/02A (3-97)
sign (+) inside this box

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DECLARATION

ADDITIONAL INVENTOR(S) Supplemental Sheet Page 1 of 1

Name of Additio	nal Joint Inventor, if a	ny:			A petitio	n has been file	d for th	is unsig	ned im	ventor	
Given Na	ume (first and middle [if any	y])	Family Name or Surname								
Eug	ene I.		0		Shakhi	novich					
Inventor's Signature								Date	,		
Residence: City	Lexington	State	МА		Country	USA		Citizen	hlp	USA	
Post Office Address 16 Woodcliffe Road											
Post Office Address								<u> </u>			-
City	Lexington	State	MA		ZIP	02173	Country	<u>. </u>	USA		
Name of Additional Joint Inventor, if any:					is unsig	ned inv	rentor				
Given Na	me (first and middle (if any	/])				Family Nar	ne or S	umame			
Inventor's Signature								Da	te		
Residence: City		State			Country			Citize	nship		
Post Office Address		_									
Post Office Address					,						_
City		State			ZIP		Count	try			
lame of Addition	nal Joint Inventor, if ar	ıy:			A petitio	n has been filed	d for thi	s unsigr	ned inv	entor	
Given Nar	me (first and middle [if any	1)				Family Nan	ne or S	urname			
Inventor's Signature								Da	te		
Residence: City		State			Country			Citize	nship		
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CONTINUT TONGOO

<u> </u>		(Supplemental	Oneety
Name	Registration Number	Name	Registration Number
James B. Lampert Wayne M. Kennard Michael J. Bevilacqua Hollie L. Baker Henry N. Wixon Anne-Louise Kerner Wayne A. Keown Michael A. Diener Donald R. Steinberg Gretchen A. Rice Peter M. Dichiara Richard A. Goldenberg Colleen Superko Scott M. Alter Barbara A. Barakat Edward D. Grieff Jason A. Reyes Rajesh Vallabh	24,564 30,271 31,091 31,321 32,073 33,523 33,923 37,122 37,241 37,429 38,005 38,895 39,850 32,879 32,190 38,898 41,513 35,761		Number

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a valid OMB control number.

DECLARATION FOR UTILITY OR DESIGN PATENT APPLICATION (37 CFR 1.63)

Declaration Submitted with Initial

 □ Declaration Submitted after Initial Filing (surcharge (37 CFR 1.16 (e)) required)

Attorney Docket Nur	iber 426.97.26	5		
First Named Invento	DeWitte			
COMPL	TE IF KNOWN			
Application Number	09 / 220,363			
Filing Date	December 24, 1998			
Group Art Unit	Not Assigned			
Examiner Name	Not Assigned			

My residence, post office a	address, and citizenship are	as stated below next to my	name.				
I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:							
System and	Method for Str	ucture-Based I	rug Desi	gn That			
Includes Accurate Prediction of Binding Free Energy							
the specification of which (Title of the Invention)							
ls attached hereto							
was filed on (MM/DI	DMM 12/24/98	as Unite	d States Applica	tion Number or F	CT International		
Application Number 09	9/220,363 and w	as amended on (MM/DD/Y	m		(if applicable).		
I hereby state that I have re amended by any amendme	viewed and understand the nt specifically referred to ab-	contents of the above identove.	tified specification	n, including the c	dalms, as .		
I acknowledge the duty to d	isclose Information which is	material to patentability as	defined in 37 Cf	R 1.56.			
I hereby claim foreign priority benefits under 35 U.S.C. 119(a)-(d) or 365(b) of any foreign application(s) for patent or inventor's certificate, or 365(a) of any PCT international application which designated at least one country other than the United States of America, listed below and have also identified below, by checking the box, any foreign application for patent or inventor's certificate, or of any PCT international application having a filling date before that of the application on which priority is claimed.							
Prior Foreign Application Number(s)	Country	Foreign Filling Date (MM/DD/YYYY)	Priority Not Claimed	Certified Co	py Attached? NO		
			0000	0000	0000		
Additional foreign application numbers are listed on a supplemental priority data sheet PTO/SB/02B attached hereto:							
I hereby claim the benefit u			application(s) lis	ted below.			
Application Number(s) Filing Date	(MM/DD/YYYY)		onal provisiona ors are listed or			
			supple	mental priority B/02B attache	data sheet		

[Page 1 of 4]

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HOPPOL TANKONOOL

DECLADATION

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I hereby clain United States United States Information wand the nation	the ber of Ame or PCT hich is n all or PC	nefit under 35 U rica, listed bek International ap naterial to pate T international	.S.C. 120 by and, in plication in ntability as filling date	of any United sofar as the in the manner defined in 3 of this applica	States applications of the state of the stat	ication(s), er of each the first p which bec	or 36: of the aragra ame	5(c) of any F e claims of ph of 35 U.S available be	CT Inte this app 5.C. 112 ween th	mation dication , I ack ne filing	al application is not disclo- nowledge the o date of the p	designating the sed in the priod duty to disclose rior application
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X Additional	registere	d practitioner(s) named o	n supplement	al Registere	d Practitio	ner in	formation sh	eet PTC)/SB/02	C attached he	ereto.
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Name		Keum	J. Pa	rk								
Address	<u> </u>	Hale	and D	orr LLP								
Address		60 St	ate S	treet								
City		Bosto	n			State		MA	ZíP	ZIP 02109		
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Name of So	le or F	irst Invento	or:			Пар	etition	has been	filed fo	r this (unsigned inv	entor
Giv	en Nar	ne (first and n	niddle [if	any])				Family	Name	or Su	mame	
		Robert	: s.				Del	Witte				
inventor's Signature						*					Date	
Residence: C	ity	Gurnee State IL Country USA Citizenship Canada					Canada					
Post Office Ad	dress	1518 A	1made	n Lane								
Post Office Ad	dress	-										·
City		Gurnee	State	IL	ZIP		031		Cou	<u> </u>	USA	
X Additional is	nventor	s are being n	amed on	theL_su	pplementa	l Addition	nal In	ventor(s) s	heet(s)	PTO/	SB/02A attac	hed hereto

valid OMB control number.

DECLARATION

ADDITIONAL INVENTOR(S) Supplemental Sheet Page 1 of 1

Name of Additio	nal Joint Inventor, if a	ny:	Į.	A petition	on has been filed	l for this	unsigned	inventor
Given Na	me (first and middle [if any	/])		Family Name or Sumame				
Eug	ene I.	,		Shakh	novich			
Inventor's Signature	886	U		\		3-	23 - 99 Date	·
Residence: City	Lexington	State	MA	Country	USA		Citizenship	USA
Post Office Address	16 Woodcliffe R	toad						
Post Office Address							,	
City	Lexington	State	MA	ZIP	02173 ر	Country	US	A
Name of Addition	nal Joint Inventor, if a	ny:	. [A petition	n has been filed	for this	unsigned	inventor
Given Na	me (first and middle (if any	1)			Family Nam	e or Su	mame	
Inventor's Signature							Date	
Residence: City		State		Country			Citizenshi	Р
Post Office Address								
Post Office Address			T					
City		State		ZIP		Countr	у	
Name of Addition	nal Joint Inventor, if ar	ıy:		A petition	n has been filed	for this	unsigned	inventor
Given Na	me (first and middle [if any	1)			Family Nam	e or Su	mame	
Inventor's Signature					<u> </u>		Date	
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P10/SIM02C (3-97)
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DECLARATION

REGISTERED PRACTITIONER INFORMATION (Supplemental Sheet)

		(Supplemental	oneet)
Name	Registration Number	Name	Registration Number
James B. Lampert Wayne M. Kennard Michael J. Bevilacqua Hollie L. Baker Henry N. Wixon Anne-Louise Kerner Wayne A. Keown Michael A. Diener Donald R. Steinberg Gretchen A. Rice Peter M. Dichiara Richard A. Goldenberg Colleen Superko Scott M. Alter Barbara A. Barakat Edward D. Grieff Jason A. Reyes Rajesh Vallabh	24,564 30,271 31,091 31,321 32,073 33,523 33,923 37,122 37,241 37,429 38,005 38,895 39,850 32,879 32,190 38,898 41,513 35,761		

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FOORBOLHBUZGBOOK

ASSIGNMENT



WHEREAS, I, Robert S. DeWitte, being a citizen of Canada, residing at 1518 Almaden Lane, Gurnee, IL 60031, and Eugene I. Shakhnovich, residing at 16 Woodcliffe Road, Lexington, MA 02173, am an inventor of certain new and useful inventions and discoveries, for which I have made an application for Letters Patent entitled System and Method for Structure-Based Drug Design That Includes Accurate Prediction of Binding Free Energy, U.S. Serial No. 09/220,363, a declaration for which I have executed on an even day; and

WHEREAS, Harvard University, a University whose address is University Place, 124 Mt. Auburn Street, Cambridge, MA 02138, and which, together with its successors and assigns is hereinafter called "ASSIGNEE," is desirous of acquiring the title, rights, benefits, and privileges hereinafter recited;

NOW, THEREFORE, for and in consideration of good and valuable consideration furnished by ASSIGNEE to me, receipt and sufficiency of which I hereby acknowledge, I hereby, without reservations:

- 1. Assign, transfer, and convey to ASSIGNEE the entire right, title, and interest in and to said inventions and discoveries, said application for Letters Patent, any and all other applications for Letters Patent on said inventions and discoveries in whatsoever countries, including all divisional, renewal, substitute, continuation, continuation-in-part, and convention applications based in whole, or in part, upon said inventions or discoveries, or upon said applications, and any and all Letters Patents, reissues, and extensions of Letters Patent granted for said inventions and discoveries or upon said applications, and every priority right that is or may be predicated upon, or arise from, said inventions, said discoveries, said applications, and said Letters Patent:
- 2. Authorize ASSIGNEE to file patent applications in any or all countries on any or all of said inventions and discoveries in my name or in the name of

ASSIGNEE or otherwise as ASSIGNEE may deem advisable, under International Conventions or otherwise;

- 3. Authorize and request the Commissioner of Patents and Trademarks of the United States of America and the empowered officials of all other governments throughout the world to issue or transfer all said Letters Patents to ASSIGNEE, as assignee of the entire right, title, and interest therein or otherwise as ASSIGNEE may direct;
- 4. Warrant that I have not knowingly conveyed to others any right in said inventions, discoveries, applications, or patents, or any license to use the same, or to make, use, or sell anything embodying or utilizing any of said inventions or discoveries; and that I have good right to assign the same to ASSIGNEE without encumbrance;
- 5. Bind my heirs, legal representatives, and assigns, as well as myself, to do, upon ASSIGNEE's request and at ASSIGNEE's expense, but without additional consideration to me or them, all acts reasonably serving to assure that said inventions and discoveries, said patent applications, and said Letters Patents shall be held and enjoyed by ASSIGNEE as fully and entirely as the same could have been held and enjoyed by me, our heirs, legal representatives, and assigns if this Assignment had not been made; and particularly to execute and deliver to ASSIGNEE all lawful application documents including petitions, specifications, and oaths, and all assignments, disclaimers, and lawful affidavits in form and substance as may be requested by ASSIGNEE; and to communicate to ASSIGNEE all facts known to me relating to said inventions and discoveries or the history thereof, and to testify as to the same in any court or proceeding; and to furnish ASSIGNEE any and all documents, photographs, models, samples, and other physical exhibits in my control or in the control of my heirs, legal representatives, or assigns which may be useful

Attorney Docket No. 426.97.265CIP

for establishing the facts of my conceptions, disclosures, and reduction to practice of said inventions and discoveries.

IN TESTIMONY WH	EREOF, I have h	ereunto set my hand	and seal.
DATE: <u>Mar 9</u> /	199	Robert S. DeWitte	
WITNESSED BY:			
Michelle K DeWite Name	Matuled	Con Dollar	
1518 Aladon Ln			
1518 Almober Lr Gunle 11 60031 Address			
DATE: Mar 9/99			
DATE:	·	Eugene I. Shakhno	vich
WITNESSED BY:			
Name			
	€.		
Address			
DATE:			

Attorney Docket No. 426.97.265CIP

for establishing the facts of my conceptions, disclosures, and reduction to practice of said inventions and discoveries.

IN TESTIMONY WHEREOF, I have hereunto set my hand and seal.

DATE:	Robert S. DeWitte
WITNESSED BY:	
Name	
Address	
DATE:	
DATE: <u>3~23~99</u>	Eugene I. Shakhnovich
WITNESSED BY:	
Patricia Gall	
Name	• .
Harvard University Mallinckrodt B9-33	
12 Oxford Street Cambridge, MA 02138	
Address	10 y 0 x
DATE: 3-23-99	